Colossal magnetoresistance in amino-functionalized graphene quantum dots at room temperature: Manifestation of weak anti-localization and doorway to spintronics

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Supplementary Information

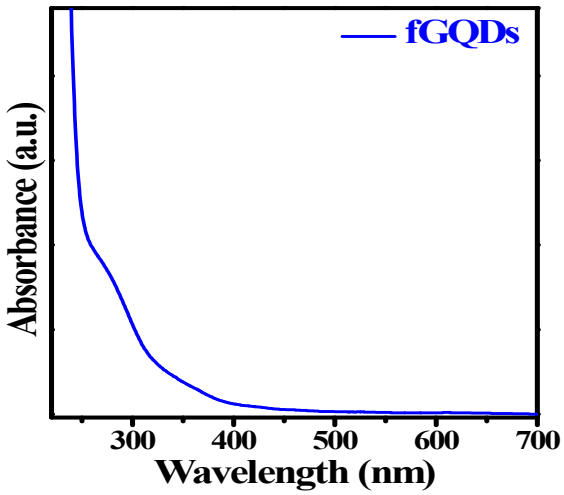

Figure S1. UV-Vis absorbance spectrum of the synthesized fGQDs

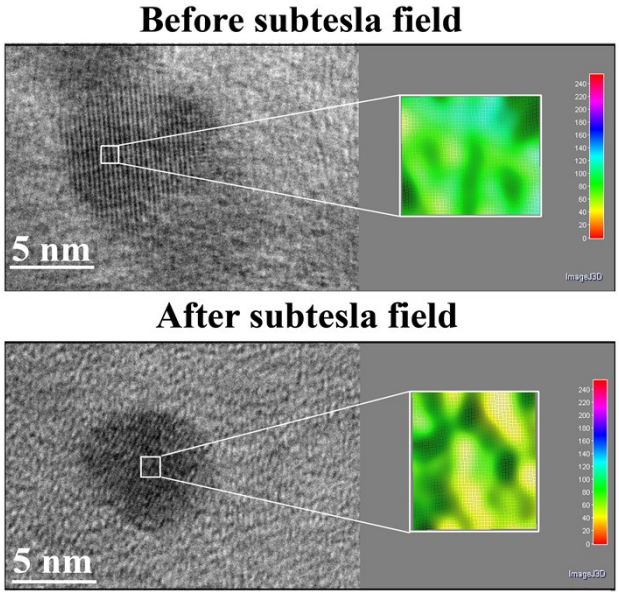

Figure S2. False-color top surface topology of lattice images corresponding to before and after the application of sTMF are reconstructed from HRTEM lattice images of fGQDs suggests the presence of deformation and on-surface ripple density accentuation in fGQDs upon sTMF exposure. The scale-bar gives an estimate of the on-surface topography fluctuations with 57.6 pixel/nm density

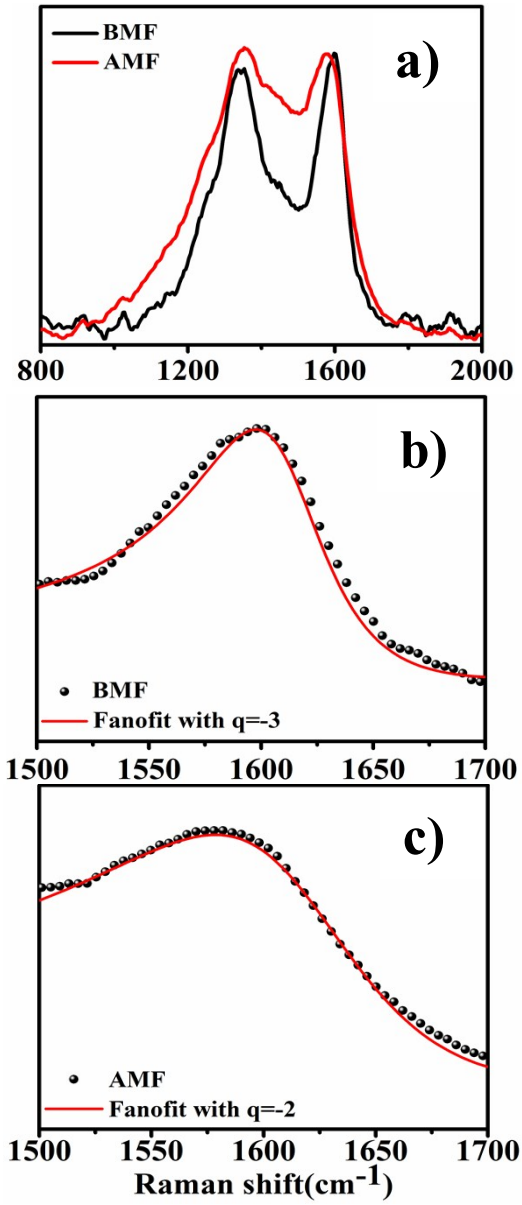

Figure S3. RAMAN spectra before and after application of the magnetic field with respective Breit-Wigner-Fano (BWF) line fitting of the G band are shown in (a, b, c)

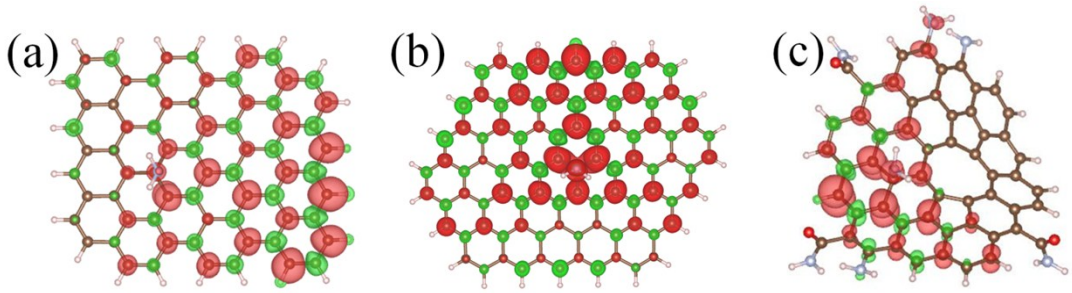

Figure S4. Spin density distribution of (a) $-NH_2$ adsorbed on Dot1 (b) DOt2 and (c) Dot3

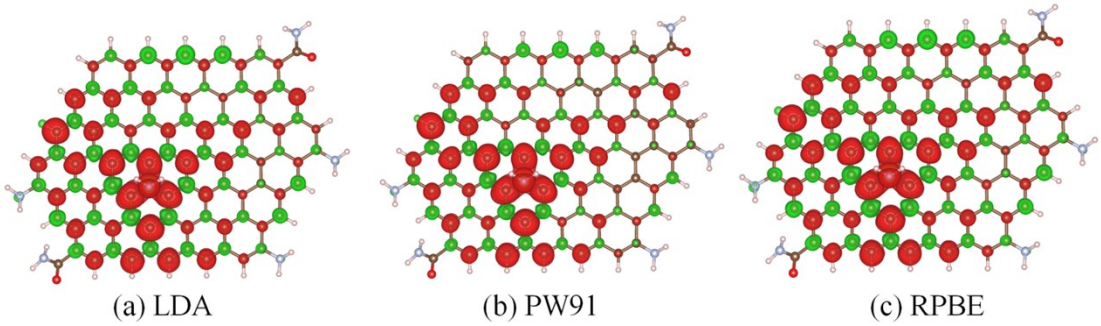

Figure S5. Spin density distribution of single $–NH_2$ adsorbed on GQD estimated using (a) LDA (b) PW91 and (c) RPBE exchange and correlation functional.

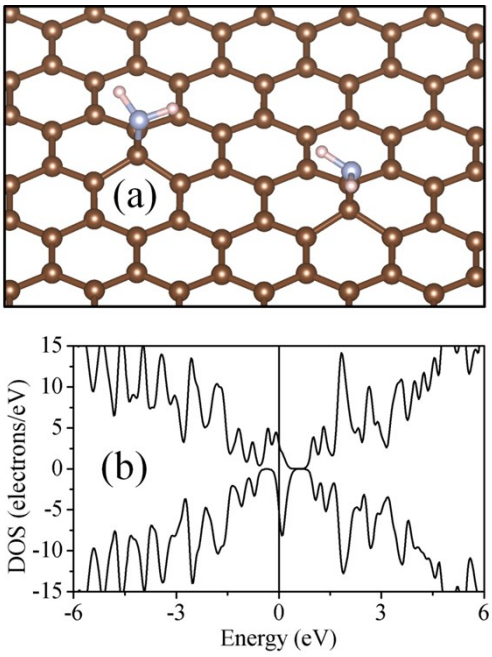

Figure S6. (a) Two NH_2 molecule adsorbed on graphene sheet (periodic structure), (b) represent corresponding spin polarized density of states.

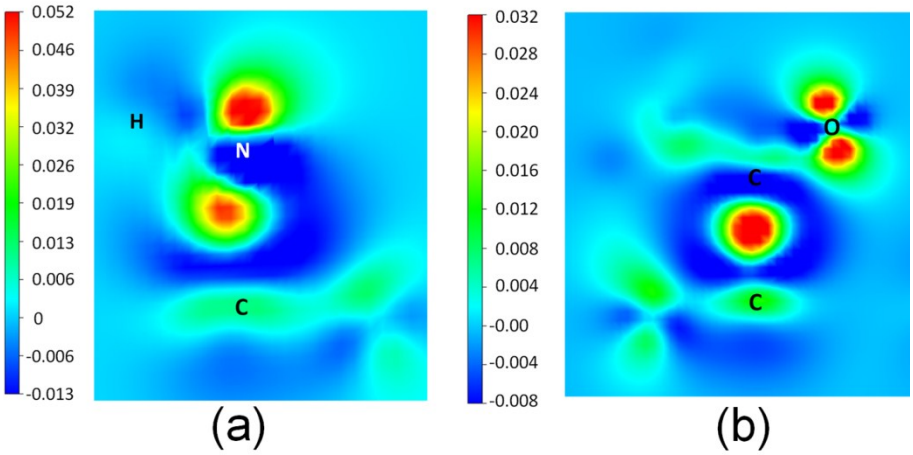

Figure S7. (a) Charge density difference 2D slice after the adsorption of (a) $–NH_2$ on GQD, (b) and O=C-NH_2 on GQD surface. The color bars represent the accumulation and depletion of charge in the considered 2D plane.

Physical insight on the nature of interaction of reactant (R) $–NH_2$ and O=C-NH_2 with the GQD surfaces can be obtained using the charge density difference ($\Delta\rho$), defined as:

$\Delta\rho = \rho(R\text{-}SiC) – \rho\ (SiC) – \rho(R)$, where

$\rho(R\text{-}GQD)$, $\rho(GQD)$ and $\rho(R)$ are the individual charge densities of the reactant ($–NH_2$ and O=C-NH_2) -adsorbed system, clean GQD surface and isolated reactant molecule respectively. The red and blue colors represent charge accumulation and charge depletion respectively and From Figure S7 (a) and S7 (b), it is evident that GQD surface undergo the charge redistribution after the adsorption of functional group, indicating tendency to adsorb the reactant. The $–NH_2$ interact with the GQD mostly via chemical bond with both ionic and covalent nature, whereas the O=C-NH_2 molecule forms mostly covalent bond with the GQD surface.

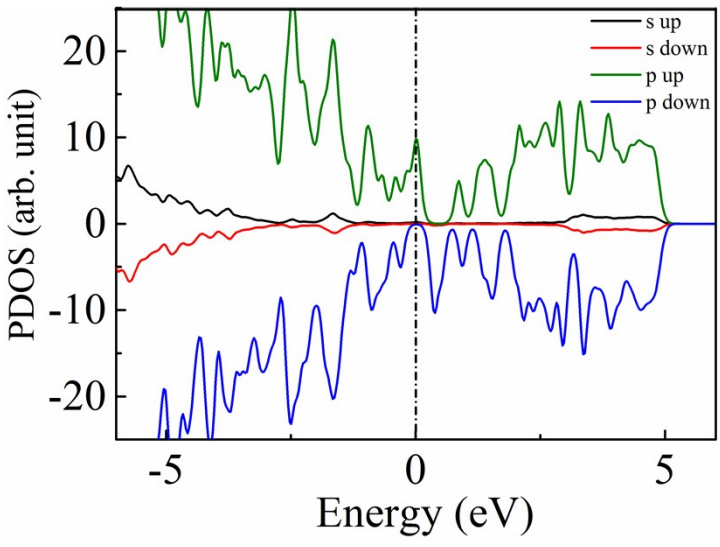

Figure S8. (a) spin polarized density of states due to presence of both two (-NH_2) and one (O=C-NH_2) functional groups over the QD surface exhibiting ~ 99% spin polarization (SP) under 0.2% strain due to increased '*a*'(e)